

# Model-based clustering of multivariate binary data with dimension reduction

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## Abstract

Clustering methods with dimension reduction have been receiving considerable wide interest in statistics lately and a lot of methods to simultaneously perform clustering and dimension reduction have been proposed. This work presents a novel procedure for simultaneously determining the optimal cluster structure for multivariate binary data and the subspace to represent that cluster structure. The method is based on a finite mixture model of multivariate Bernoulli distributions, and each component is assumed to have a low-dimensional representation of the cluster structure. This method can be considered an extension of the traditional latent class analysis model. Sparsity is introduced to the loading values, which produces the low-dimensional subspace, for enhanced interpretability and more stable extraction of the subspace. An EM-based algorithm is developed to efficiently solve the proposed optimization problem. We demonstrate the effectiveness of the proposed method by applying it to a simulation study and real datasets.

Key words: Binary data; Clustering; Dimension reduction; EM algorithm; Latent class analysis; Sparsity

## 1 Introduction

Binary data are commonly observed and analyzed in many application fields: behavioral and social research, biosciences, document classification, and inference on binary images. For example, Ekholm et al. (2000) analyzed biomedical data including five unequally spaced binary self-assessment measurements of arthritis and obesity data on the presence or absence of obesity in five cohorts of children. Also, the binarized data of the MovieLens 100K and the Netflix dataset, which are popular datasets for collaborative filtering tasks, have been analyzed by Kozma et al. (2009). One of the purposes of analyzing binary data, as well as continuous data, is the partitioning of binary objects into several unpredetermined homogeneous groups (clusters). For clustering of multivariate data, it is quite important to know if some of the variables do not contribute much to the structure of clusters because the inclusion of redundant information can reduce the performance of the cluster analysis (Milligan, 1996). Also, a lower-dimensional (say two or three dimensional) representation of the cluster structure, based on the most significant information, is very useful for evaluating and interpreting the results of the cluster analysis.

Hence, what is needed is a procedure that constructs a low-dimensional representation of the multivariate binary data, such that the cluster structure in the data is maximally revealed. For this purpose, researchers often carry out a preliminary dimension reduction technique (e.g., Collins et al., 2002; Schein et al., 2003; Lee et al., 2010). Cluster analysis is then performed on the object scores on the first few principal components. Although it is easy to implement, this two-step sequential approach, also called the tandem approach, provides no assurance that the components extracted in the first

step are optimal for the subsequent cluster analysis, because the two steps are implemented separately by optimizing a different loss function (Arabie and Hubert, 1994; DeSarbo et al., 1990; De Soete and Carroll, 1994; Vichi and Kiers, 2001; Timmerman et al., 2010; Yamamoto and Hwang, 2014). For multivariate continuous data, instead of the two-step tandem clustering procedure, several methods that simultaneously perform cluster analysis and dimension reduction have been proposed (De Soete and Carroll, 1994; Vichi and Kiers, 2001; Ghahramani and Hinton, 1997; Yoshida et al., 2004).

On the other hand, for multivariate binary data, a few methods can conduct the analysis for simultaneously obtaining a cluster structure and a subspace for the cluster structure. Patrikainen and Mannila (2004) have developed a subspace clustering method of binary data that can be used in high-dimensional settings. Bouguila (2010) has developed a clustering method for multivariate binary data with feature weighting that allows variable selection taking variables with large weights. Recently, Wu (2013) has proposed a penalized latent class model for clustering extremely large-scale discrete data. This method can be also considered a weighting method. Cagnone and Viroli (2012) have proposed a factor mixture analysis model for multivariate binary data, in which latent variables are distributed as a finite mixture of multivariate Gaussian distributions.

In this paper, we focus on the common subspace clustering in which a cluster structure is present in a low-dimensional space. As described above, Patrikainen and Mannila’s (2004) method allows for obtaining a cluster structure and a subspace for the cluster structure simultaneously. However, their method is rather cluster-specific subspace clustering. In addition, in the past few decades, because of technical advances in storing and processing data, we can obtain a large dataset that includes a large number of variables. Thus, we need to take into account such high-dimensional data. In a high-dimensional setting, weighting methods for high-dimensional data, such as those of Bouguila (2010) and Wu (2013), may be promising because variables that have lower weights are suggested for exclusion from the model. However, their methods do not provide explicit low-dimensional representation of the data, which is useful for evaluating and interpreting the cluster structure. Thus, in this paper, we propose a new method to simultaneously find a cluster structure of multivariate binary data and an optimal low-dimensional space for clustering. Furthermore, our proposed method can deal with high-dimensional data.

The remainder of this paper is structured as follows. In Section 2, we propose a new method to cluster multivariate binary data with dimension reduction. Section 3 describes an algorithm for the proposed optimization problem. Section 4 is devoted to studying the working of the clustering method using artificial and real data examples. Finally, we sum up our findings and set out directions for future expansion in Section 5.

## 2 Proposed method

Let  $\tilde{\mathbf{y}} = (\tilde{y}_1, \dots, \tilde{y}_D)'$  be a random vector of  $D$  binary variables. Suppose there are  $K$  latent (unobservable) classes in a population and let  $\tilde{u}_k$ ,  $k = 1, \dots, K$ , be an allocation variable that takes “1” if an observation belongs to class  $k$ , and “0” otherwise. We

write  $\tilde{\mathbf{u}} = (\tilde{u}_1, \dots, \tilde{u}_K)'$ . We assume that the allocation variable follows a multinomial distribution, i.e., the probability that  $\tilde{\mathbf{u}}$  takes the value  $\mathbf{u} = (u_1, \dots, u_K)'$  is

$$f(\tilde{\mathbf{u}} = \mathbf{u}) = \prod_{k=1}^K \xi_k^{u_k},$$

where  $\xi_k = \Pr(\tilde{u}_1 = 0, \dots, \tilde{u}_k = 1, \dots, \tilde{u}_K = 0)$ .

Given that an observation is in the  $k$ th latent class, the probability that the random vector  $\tilde{\mathbf{y}}$  takes the value  $\mathbf{y} = (y_1, \dots, y_D)'$ , where each  $y_d$  takes 0 or 1, is represented as  $\Pr(\tilde{\mathbf{y}} = \mathbf{y} \mid \tilde{u}_k = 1)$ . The unconditional probability of the response  $\mathbf{y}$  when we do not know the latent class of the observation is

$$\Pr(\tilde{\mathbf{y}} = \mathbf{y}) = \sum_{k=1}^K \xi_k \Pr(\tilde{\mathbf{y}} = \mathbf{y} \mid \tilde{u}_k = 1). \quad (1)$$

Here, we need to specify how the probability  $\Pr(\tilde{\mathbf{y}} = \mathbf{y} \mid \tilde{u}_k = 1)$  depends on parameters. We postulate that, given the latent class to which an observation belongs, the responses on the binary variables are independent:

$$\Pr(\tilde{\mathbf{y}} = \mathbf{y} \mid \tilde{u}_k = 1) = \prod_{d=1}^D \Pr(\tilde{y}_d \mid \tilde{u}_k = 1). \quad (2)$$

This assumption of *conditional independence* has been widely used in latent class modeling in sociology (Collins and Lanza, 2010), and is directly analogous to the assumption in the factor analysis model that observed variables are conditionally independent given the factors (Aitkin et al., 1981).

Finally, to specify the model completely, we need to specify a set of parameters that define the conditional probability of  $\tilde{\mathbf{y}}$ , with the value of  $\tilde{\mathbf{u}}$  given. Suppose that  $\tilde{\mathbf{y}}_1, \dots, \tilde{\mathbf{y}}_N$  are mutually independent random variables that have the same distribution as  $\tilde{\mathbf{y}}$ , and the entries of  $\mathbf{Y} = (y_{nd})$  are those realizations. We assume that, given the class  $k$ ,  $\tilde{y}_d$  follows the Bernoulli distribution with success probability  $\pi_{kd}$ . For the traditional latent class analysis model (Aitkin et al., 1981), we consider a parameter vector  $\boldsymbol{\theta}_k = (\theta_{k1}, \dots, \theta_{kD})'$ , where  $\theta_{kd}$  is the logit transformation of  $\pi_{kd}$ . We define the inverse logit transformation  $\pi(\theta) = \{1 + \exp(-\theta)\}^{-1}$ . The success probabilities can be represented using the canonical parameters  $\theta_{kd}$  as  $\pi_{kd} = \pi(\theta_{kd})$ . Let  $\tilde{y}_{nd}$  be the  $d$ th element of  $\tilde{\mathbf{y}}_n$ . The individual data-generating probability given the class then becomes

$$\begin{aligned} \Pr(\tilde{y}_{nd} = y_{nd} \mid \tilde{u}_k = 1) &= \Pr(\tilde{y}_{nd} = y_{nd} \mid \tilde{u}_k = 1, \theta_{kd}) \\ &= \pi(\theta_{kd})^{y_{nd}} \{1 - \pi(\theta_{kd})\}^{1-y_{nd}} \\ &= \pi(q_{nd}\theta_{kd}), \end{aligned}$$

with  $q_{nd} = 2y_{nd} - 1$  since  $\pi(-\theta) = 1 - \pi(\theta)$ . Then, these representations lead to the compact form of the log likelihood as

$$\sum_{n=1}^N \log \left( \sum_{k=1}^K \xi_k \prod_{d=1}^D \pi(q_{nd}\theta_{kd}) \right).$$

We aim to obtain a low-dimensional representation of binary data in which the true cluster structure exists. Thus, we assume that canonical parameter  $\theta_{kd}$  has a low-rank representation as follows:

$$\theta_{kd} = \mu_d + \mathbf{f}_k' \mathbf{a}_d, \quad (3)$$

where  $\mu_d \in \mathbb{R}$ , and for some positive integer  $L$ ,  $\mathbf{f}_k \in \mathbb{R}^L$  and  $\mathbf{a}_d \in \mathbb{R}^L$ . Here,  $\mu_d$ ,  $\mathbf{f}_k$ , and  $\mathbf{a}_d$  denote a centroid for the  $d$ th variable, a component score of the  $k$ th cluster, and a loading value for the  $d$ th variable, respectively. We write  $\boldsymbol{\xi} = (\xi_1, \dots, \xi_K)'$ ,  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_D)'$ ,  $\mathbf{F} = (\mathbf{f}_1, \dots, \mathbf{f}_K)'$ , and  $\mathbf{A} = (\mathbf{a}_1, \dots, \mathbf{a}_D)'$ . To guarantee identifiability, we require that  $\mathbf{F}$  has orthonormal columns. Then the log likelihood can be written as

$$\ell(\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) = \sum_{n=1}^N \log \left( \sum_{k=1}^K \xi_k \prod_{d=1}^D \pi(q_{nd}(\mu_d + \mathbf{f}_k' \mathbf{a}_d)) \right). \quad (4)$$

Here, to deal with the high-dimensional problem, we assume that most of the elements of the true  $\mathbf{A}$  are exactly zero. A sparse loading matrix implies variable selection in cluster analysis. That is, variables with non-zero loadings can be considered to contribute to a cluster structure in a low-dimensional space, whereas variables with zero loadings have no effect on the cluster structure. We propose to perform variable selection using the penalized likelihood with sparsity-inducing penalties. If  $K = 1$  and  $\mathbf{f}_k$  is observable, Eq. (4) is the log likelihood for  $D$  logistic regression models. This connection with logistic regression suggests the use of the  $L_1$  penalty to obtain a sparse loading matrix, as in the Lasso regression (Tibshirani, 1996). Specifically, consider the penalty

$$P_\lambda(\mathbf{A}) = \sum_{l=1}^L \lambda_l \|\tilde{\mathbf{a}}_l\|_{L_1} = \lambda_1 \sum_{d=1}^D |a_{d1}| + \dots + \lambda_L \sum_{d=1}^D |a_{dL}|,$$

where  $\tilde{\mathbf{a}}_l$  denotes the  $l$ th column of  $\mathbf{A}$  and  $\lambda_l$  is a regularization parameter. The choice of values for  $\lambda_l$  will be discussed later. We obtain cluster components  $\boldsymbol{\xi}$ ,  $\boldsymbol{\mu}$ , and  $\mathbf{F}$  and a sparse loading matrix  $\mathbf{A}$  by maximizing the following penalized log likelihood:

$$S(\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) = \ell(\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) - N \cdot P_\lambda(\mathbf{A}). \quad (5)$$

We call this procedure the clustering of binary data with reducing the dimensionality (CLUSBIRD). We can interpret penalized maximization as the device for generating a suitable optimization function, but not a realistic representation of the actual data-generating process. Thus, in this sense, the conditional independence given the latent class for obtaining the likelihood in Eq. (4) is assumed. A computational algorithm for solving the maximization problem is presented in the next section.

The effectiveness of the introduction of sparsity is illustrated in Figure 1 using a rank-two model (i.e.,  $L = 2$ ). The details of the setting will be presented in Section 4. While the regularized model can recover the original loading vector efficiently under the sparsity assumption, the unregularized model gives more noisy results. In the context of the ordinary factor analysis model, a sparse structure for the loading matrix provides an easy interpretation of the result, whereas it is difficult to interpret the relation between

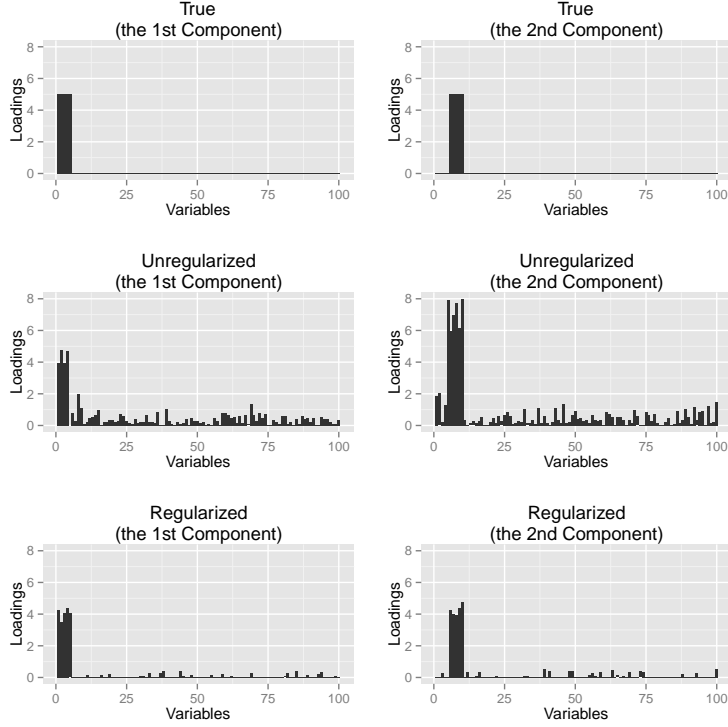


Figure 1: The results of analyzing an artificial dataset with  $N = 100$ ,  $D = 100$ ,  $L = 2$ , and  $K = 4$ ; top, middle, and bottom panels show the true loadings, absolute values of loadings from the unregularized model, and absolute values of loadings from the regularized model, respectively; left and right panels show loadings for the first and second components, respectively; the penalty parameter was selected using the Bayesian information criterion

variables and factors if the loading matrix has no sparse structure. Browne (2001) provides an excellent overview of the sparsity and rotation techniques which aim to obtain a sparse structure. In addition, Hirose and Yamamoto (2014) discuss the sparsity problem in the factor analysis model. Similar to the ordinary factor analysis model, noisy loading values may lead to difficulty in the interpretation of the result in our model. Thus, for the proposed model, sparse loading values offer an advantage.

### 3 Optimization Algorithm

As is often the case, we apply the EM algorithm (Dempster et al., 1977) to solve the maximization problem (5). Let  $\mathbf{U} = (u_{nk})$  be  $N$  realizations of mutually independent random variable  $\tilde{\mathbf{u}}$ . In addition, denote the conditional probability (2) by  $p_k(\mathbf{y} \mid \boldsymbol{\theta}_k)$ .

Then, the complete-data likelihood can be written as follows:

$$L^C(\mathbf{Y}, \mathbf{U} \mid \boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) = \prod_{n=1}^N \left\{ \prod_{k=1}^K p_k(\mathbf{y}_n \mid \boldsymbol{\theta}_k)^{u_k} \prod_{k=1}^K \xi_k^{u_k} \right\}.$$

As described in the previous section, we aim to obtain the sparse loading matrix  $\mathbf{A}$ ; therefore, the penalty term for sparsity should be introduced. Thus, the complete-data log-likelihood with the penalty is

$$\ell^C(\mathbf{Y}, \mathbf{U} \mid \boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) = \sum_{n=1}^N \sum_{k=1}^K u_{nk} \log p_k(\mathbf{y}_n \mid \boldsymbol{\theta}_k) + \sum_{n=1}^N \sum_{k=1}^K u_{nk} \log \xi_k - N \cdot P_\lambda(\mathbf{A}). \quad (6)$$

The EM algorithm consists of a step maximizing the conditional expectation of the complete-data log-likelihood function (6) given the observable data  $\mathbf{Y}$  and a set of parameters,  $\{\boldsymbol{\xi}^{(t)}, \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)}\}$ . Here,  $\boldsymbol{\xi}^{(t)}$  denotes the value of  $\boldsymbol{\xi}$  at the  $t$ th step in the algorithm, and this notation is applied to other parameters. From the above formulation, we can see that the penalized complete-data log-likelihood (6) is a linear function with respect to values of  $u_{nk}$ . Thus, to obtain the conditional expected value of  $\ell^C$ , we only have to replace  $u_{nk}$  with its conditional expectation,

$$\begin{aligned} u_{nk}^* &:= E \left[ u_{nk} \mid \mathbf{Y}; \boldsymbol{\xi}^{(t)}, \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)} \right] \\ &= \frac{\xi_k^{(t)} p_k(\mathbf{y}_n \mid \boldsymbol{\theta}_k^{(t)})}{\sum_{k=1}^K \xi_k^{(t)} p_k(\mathbf{y}_n \mid \boldsymbol{\theta}_k^{(t)})}, \end{aligned} \quad (7)$$

where  $\boldsymbol{\theta}_k^{(t)} = (\theta_{k1}^{(t)}, \dots, \theta_{kD}^{(t)})'$ ,  $k = 1, \dots, K$ , is obtained through Eq. (3) using  $\{\boldsymbol{\xi}^{(t)}, \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)}\}$ . Thus, the conditional expectation of the complete-data log-likelihood is as follows:

$$\begin{aligned} Q(\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A} \mid \boldsymbol{\xi}^{(t)}, \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)}) &= E \left[ \ell^C \mid \mathbf{Y}; \boldsymbol{\xi}^{(t)}, \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)} \right] \\ &= \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* \log p_k(\mathbf{y}_n \mid \boldsymbol{\theta}_k) + \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* \log \xi_k - N \cdot P_\lambda(\mathbf{A}). \end{aligned}$$

In the M-step of the EM algorithm, we consider the following maximization problem

$$(\hat{\boldsymbol{\xi}}, \hat{\boldsymbol{\mu}}, \hat{\mathbf{F}}, \hat{\mathbf{A}}) = \arg \max_{\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}} Q(\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A} \mid \boldsymbol{\xi}^{(t)}, \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)}). \quad (8)$$

Same as the usual mixture models, the estimate of  $\boldsymbol{\xi}$  can be obtained by

$$\hat{\xi}_k = N^{-1} \sum_{n=1}^N u_{nk}^*, \quad \text{for } k = 1, \dots, K-1, \quad (9)$$

and  $\hat{\xi}_K = 1 - \sum_{k=1}^{K-1} \hat{\xi}_k$ .

Given the estimate of  $\boldsymbol{\xi}$ , the maximization problem in (8) with respect to  $\boldsymbol{\mu}$ ,  $\mathbf{F}$ , and  $\mathbf{A}$  is equivalent to the minimization of the following function:

$$g(\boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) = - \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* \log p_k(\mathbf{y}_n | \boldsymbol{\theta}_k) + N \cdot P_\lambda(\mathbf{A}). \quad (10)$$

Here, the function  $g$  in (10) is non-quadratic. Then, instead of directly dealing with the non-quadratic function  $g$ , we minimize a surrogate function, called the majorizing function (Hunter and Lange, 2004), to solve the minimization problem of a quadratic function. In the majorization algorithm, a suitably defined quadratic upper bound of (10) is minimized, which provides optimal values for the actual function  $m$ . A function  $h(x | y)$  is said to majorize a function  $m(x)$  at  $y$  if

$$h(x | y) \geq m(x) \quad \text{for all } x \quad \text{and} \quad h(y | y) = m(y).$$

In the geometrical view, the function surface  $h(x | y)$  lies above the function  $m(x)$  and is tangent to it at the point  $y$ ; therefore  $h(x | y)$  becomes an upper bound of  $m(x)$ . To minimize  $m(x)$ , the majorization algorithm decreases the objective function  $m(x)$  in each step and is guaranteed to converge to a local minimum of  $m(x)$ . When applying the majorization algorithm, the majorizing function  $h(x | y)$  is chosen so that it is easier to minimize than the original objective function  $m(x)$ . The study by Hunter and Lange (2004) can be referred for an introductory description of the majorization algorithm.

To find a suitable majorizing function of (10), we consider the first term of (10). Note that, for a given point  $y$ ,

$$-\log \pi(x) \leq -\log \pi(y) - \{1 - \pi(y)\}(x - y) + \frac{1}{8}(x - y)^2, \quad (11)$$

and the equality holds when  $x = y$  (Jaakkola and Jordan, 2000; De Leeuw, 2006). This equation provides quadratic upper bounds for the first term of (10) at the tangent point  $y$ . Thus we can apply the majorization algorithm for our problem.

We now present details of the majorization algorithm via the upper bound of  $-\log \pi(x)$  in (11). By completing the square, Eq. (11) can be rewritten as

$$-\log \pi(x) \leq -\log \pi(y) + \frac{1}{8} [x - y - 4\{1 - \pi(y)\}]^2. \quad (12)$$

Substituting  $x$  and  $y$  with  $q_{nd}\theta_{kd}$  and  $q_{nd}\theta_{kd}^{(t)}$ , respectively in (12) and using  $q_{nd} = \pm 1$ , we obtain

$$-\log \pi(q_{nd}\theta_{kd}) \leq -\log \pi(q_{nd}\theta_{kd}^{(t)}) + \frac{1}{8} (\theta_{kd} - z_{nkd}^{(t)})^2, \quad (13)$$

where

$$z_{nkd}^{(t)} = \theta_{kd}^{(t)} + 4q_{nd} \left\{ 1 - \pi(q_{nd}\theta_{kd}^{(t)}) \right\}.$$



Thus, we obtain the following quadratic upper bound of the first term of (10):

$$\frac{1}{8} \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* \sum_{d=1}^D (\theta_{kd} - z_{nk d}^{(t)})^2. \quad (14)$$

Eq. (14) then yields the following upper bound (up to a constant) of the criterion function  $g(\boldsymbol{\mu}, \mathbf{F}, \mathbf{A})$  defined in (10):

$$\begin{aligned} h(\boldsymbol{\mu}, \mathbf{F}, \mathbf{A} \mid \boldsymbol{\mu}^{(t)}, \mathbf{F}^{(t)}, \mathbf{A}^{(t)}) \\ = \frac{1}{8} \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* \| \mathbf{z}_{nk}^{(t)} - (\boldsymbol{\mu} + \mathbf{A} \mathbf{f}_k) \|^2 + N \cdot P_\lambda(\mathbf{A}), \end{aligned} \quad (15)$$

where  $\mathbf{z}_{nk}^{(t)} = (z_{nk1}^{(t)}, \dots, z_{nkD}^{(t)})'$ .

The majorizing function given in (15) is quadratic in each of  $\boldsymbol{\mu}$ ,  $\mathbf{F}$ , and  $\mathbf{A}$  when the other two are fixed, and thus alternating minimization of (15) with respect to  $\boldsymbol{\mu}$  and  $\mathbf{A}$  has closed-form solutions. We now drop the subscript  $(t)$  for notational convenience. For fixed  $\mathbf{F}$  and  $\mathbf{A}$ , set  $\bar{z}_{kd} = N_k^{-1} \sum_{n=1}^N u_{nk}^* z_{nk d}$  where  $N_k = \sum_{n=1}^N u_{nk}^*$ , and write  $\bar{\mathbf{z}}_k = (\bar{z}_{k1}, \dots, \bar{z}_{kD})'$ . Then the optimal  $\hat{\boldsymbol{\mu}}$  is given by

$$\begin{aligned} \hat{\boldsymbol{\mu}} &= \arg \min_{\boldsymbol{\mu}} \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* \| \mathbf{z}_{nk} - (\boldsymbol{\mu} + \mathbf{A} \mathbf{f}_k) \|^2 \\ &= N^{-1} \sum_{k=1}^K N_k (\bar{\mathbf{z}}_k - \mathbf{A} \mathbf{f}_k). \end{aligned} \quad (16)$$

Optimization of  $\mathbf{F}$  requires a numerical procedure because of its orthonormality. To update  $\mathbf{F}$  for fixed  $\boldsymbol{\mu}$  and  $\mathbf{A}$ , we apply the gradient projection (GP) algorithm with the orthonormal constraint (Jennrich, 2001, 2002). The only problem specific thing required for the GP algorithm is the gradient of (15) viewed as a function of  $\mathbf{F}$ . Let  $\bar{z}_{kd}^* = N_k^{-1} \sum_{n=1}^N u_{nk} (z_{nk d} - \mu_d)$ , and write  $\bar{\mathbf{Z}}^* = (\bar{z}_{kd}^*)$ . Furthermore, let  $\mathbf{N}$  be a  $K \times K$  diagonal matrix where the  $k$ th diagonal element is  $N_k$ . Then, the gradient of  $h$  at  $\mathbf{F}$  is given as follows:

$$\boldsymbol{\Gamma} = \frac{\partial h}{\partial \mathbf{F}} = \frac{1}{4} \mathbf{N} (\mathbf{F} \mathbf{A}' - \bar{\mathbf{Z}}^*) \mathbf{A}. \quad (17)$$

Using  $\boldsymbol{\Gamma}$  as the gradient in the GP algorithm with orthonormal constraint, we obtain the optimal  $\hat{\mathbf{F}}$ .

Finally, for fixed  $\boldsymbol{\mu}$  and  $\mathbf{F}$ , the  $dl$ th element  $a_{dl}$  of  $\mathbf{A}$  is updated by solving the minimization problem in (15) directly. Let  $v_{dl} = \sum_{n=1}^N \sum_{k=1}^K u_{nk}^* (z_{nk d} - \mu_d) f_{kl}$  and  $w_{ll'} = \sum_k N_k f_{kl} f_{kl'}$ . Then, up to a constant, the loss function with respect to  $\mathbf{A}$  can be written as

$$h'(\mathbf{A}) = \frac{1}{8} \sum_{d=1}^D \sum_{l=1}^L \sum_{l'=1}^L w_{ll'} a_{dl} a_{dl'} - \frac{1}{4} \sum_{d=1}^D \sum_{l=1}^L v_{dl} a_{dl} + N \sum_{l=1}^L \lambda_l \sum_{d=1}^D |a_{dl}|. \quad (18)$$

Let  $s_{dl} = \text{sign}(a_{dl})$  for  $a_{dl} \neq 0$ , and  $s_{dl} \in [-1, 1]$  for  $a_{dl} = 0$ . Thus, the subdifferential  $\partial h'_{dl}(\mathbf{A})$  of  $h'(\mathbf{A})$  at  $a_{dl}$  is as follows:

$$\partial h'_{dl}(\mathbf{A}) = \left\{ \frac{1}{4} \sum_{l'=1}^L w_{ll'} a_{dl'} - \frac{1}{4} v_{dl} + N \lambda_l s_{dl} \right\}. \quad (19)$$

Then, the optimal  $\hat{a}_{dl}$  can be obtained by

$$\hat{a}_{dl} = \frac{1}{w_{ll}} \text{sign}(c_{dl}) \max(0, |c_{dl}| - 4N\lambda_l), \quad (20)$$

where  $c_{dl} = -\sum_{l' \neq l} a_{dl'} + v_{dl}$ .

The procedure of the proposed optimization algorithm is summarized as follows:

*STEP1.* Set  $t = 1$  and initial values of  $\boldsymbol{\xi}^{(1)}$ ,  $\boldsymbol{\mu}^{(1)}$ ,  $\mathbf{F}^{(1)}$ , and  $\mathbf{A}^{(1)}$ .

*STEP2.* Calculate the conditional expectation of  $u_{nk}$  using (7).

*STEP3.* Update  $\boldsymbol{\xi}$  using (9) and set  $\boldsymbol{\xi}^{(t+1)} = \hat{\boldsymbol{\xi}}$ .

*STEP4.* Update  $\boldsymbol{\mu}$  using (16) and set  $\boldsymbol{\mu}^{(t+1)} = \hat{\boldsymbol{\mu}}$ .

*STEP5.* Update  $\mathbf{F}$  by the GP algorithm with the gradient  $\boldsymbol{\Gamma}$  in (17) and set  $\mathbf{F}^{(t+1)} = \hat{\mathbf{F}}$ .

*STEP6.* Update  $\mathbf{A}$  using (20) and set  $\mathbf{A}^{(t+1)} = \hat{\mathbf{A}}$ .

*STEP7.* Increase the value of  $t$  by 1 and repeat STEP2-6 until the penalized log-likelihood (5) converges.

Prior to applying the above algorithm, the value of the regularization parameters,  $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_L)'$ , should be determined. In regression analysis, the degree of freedom for the shrinkage method (Zou et al, 2007; Hirose et al., 2013) may be used for selecting the model selection criteria. In this paper, we choose  $\boldsymbol{\lambda}$  by minimizing the following Bayesian information criterion (BIC):

$$\text{BIC}(\boldsymbol{\lambda}) = -2\ell(\boldsymbol{\xi}, \boldsymbol{\mu}, \mathbf{F}, \mathbf{A}) + (\log N) \text{df}(\boldsymbol{\lambda}), \quad (21)$$

where  $\text{df}(\boldsymbol{\lambda})$  is the number of nonzero parameters for fixed  $K$  and  $L$ . The degree of freedom  $\text{df}(\boldsymbol{\lambda})$  used in Eq. (21) is defined as  $\text{df}(\boldsymbol{\lambda}) = K + D + KL + |\mathbf{A}|_{\boldsymbol{\lambda}}$ , where  $K$  and  $D$  are the length of the vector  $\boldsymbol{\xi}$  and  $\boldsymbol{\mu}$ , respectively,  $KL$  is the total number of elements of  $\mathbf{F}$ , and  $|\mathbf{A}|_{\boldsymbol{\lambda}}$  is the number of nonzero elements of  $\mathbf{A}$  when the regularization parameter is  $\boldsymbol{\lambda}$ . In the following sections, we use the above BIC to choose  $\boldsymbol{\lambda}$  in the proposed method. In addition, although different parameters can be used for different component loading vectors, we consider using only a single regularization parameter  $\lambda$  for all loadings.

## 4 Numerical examples

### 4.1 A Monte Carlo simulation

We conducted a simulation study to evaluate the performance of the proposed method, compared with tandem analysis (TA), in which sparse logistic principal component analysis (SLPCA) (Lee et al., 2010) is conducted, followed by the ordinary  $k$ -means clustering of estimated principal component scores.

The artificial data  $\mathbf{Y}$  were generated through the CLUSBIRD model (1) with three clusters ( $K = 3$ ) and two dimensional structure ( $L = 2$ ). That is, an object  $y_{nd}$  that was assigned to cluster  $k$  was generated by  $y_{nd} \sim \text{Ber}(\pi_{kd})$ . To determine the value of  $\pi_{kd}$ , the values of  $\boldsymbol{\mu}$ ,  $\mathbf{F}$ , and  $\mathbf{A}$  were generated. We used a zero vector for  $\boldsymbol{\mu}$ . Each centroid  $\mathbf{f}_k$  of clusters in the two-dimensional space were randomly generated so that the distance between two clusters was equal for all combinations of two clusters, and then the  $\mathbf{F} = (\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3)$  was orthonormalized. The loading matrix  $\mathbf{A}$  was set at

$$\mathbf{A} = \begin{pmatrix} c \cdot \mathbf{1}_{D_1} & \mathbf{0}_{D_1} \\ \mathbf{0}_{D_1} & c \cdot \mathbf{1}_{D_1} \\ \mathbf{0}_{D_2} & \mathbf{0}_{D_2} \end{pmatrix},$$

where  $\mathbf{1}_m$  and  $\mathbf{0}_m$  denote  $m$ -vectors of ones and zeroes, respectively. Here,  $c$  is a scalar whose value was determined based on sample size as described below. In this simulation study, we considered three factors: sample size ( $N = 100, 300$ ), the number of variables ( $D = 10, 1000$ ), and the proportion of informative variables on the cluster structure ( $m = 0.5, 1.0$ ). Then, we set the value of  $c$  was set at 2.5 for  $D = 10$  and 0.5 for  $D = 1000$ . The number  $D_1$  was calculated as  $D_1 = \lfloor \frac{m}{2} D \rfloor$ , where  $\lfloor \cdot \rfloor$  denotes a floor function. Thus, based on the above structure of  $\mathbf{A}$ ,  $2D_1$  variables contributes the low-dimensional structure and  $D_2 (= D - 2D_1)$  variables are random error variables. For each condition, we generated 50 replications, thus yielding  $2 \times 2 \times 2 \times 50 = 400$  random samples in total. We used the Adjusted Rand Index (ARI) (Hubert and Arabie, 1985) to assess the recovery of cluster memberships. The ARI has a maximal value of 1 in the case of a perfect recovery of the underlying cluster structure, and a value of 0 in the case where the true and estimated class assignments coincide no more than would be expected by chance.

In this study, we used 50 sets of random initial values of all parameters for the proposed model and SLPCA, except that initial values of  $\boldsymbol{\mu}$  in the proposed model and low-dimensional means in SLPCA were both set at zero. Also, we used the parameter values of  $K$  and  $L$  as their values, i.e., values of 3 and 2, respectively, for the two models. The values of tuning parameter  $\lambda$  in the SLPCA model were determined by BIC as defined in Lee et al. (2010). To reduce computational burden, we selected the values of tuning parameters only in the first replication for each condition, and then used the values of the parameter obtained from the selection by BIC for the remaining replications.

Figure 2 shows boxplots of the ARIs obtained from the two methods, along with the values of  $D$ ,  $m$ , and  $N$ . Each boxplot denotes the values of ARIs for 50 replications

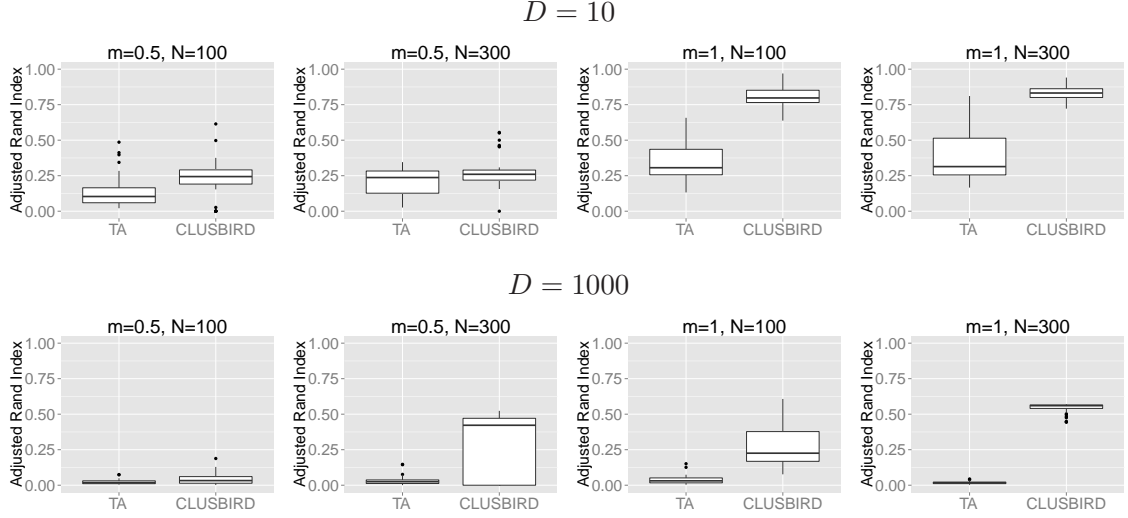


Figure 2: Boxplots of adjusted Rand indices



Figure 3: Examples of normalized bitmaps

under each condition. When the number of variables is small ( $D = 10$ ), the proposed method provided better results than tandem analysis under all cases. We can see that the recovery of the cluster structure became better when the sample size and/or the proportion of the informative variables increased. Also, under the moderately high-dimensional settings ( $D = 1000$ ), the recoveries of the proposed method were superior or similar to those of tandem analysis. Specifically, tandem analysis did not work well under the conditions with  $D = 1000$ .

## 4.2 Binary image classifications

Handwritten digit recognition has many application scenarios such as auto-mail classification according to zip code and signature recognition (Bouguila, 2010). We used binary image data that were available from the well-known UCI database (Bache and Lichman,

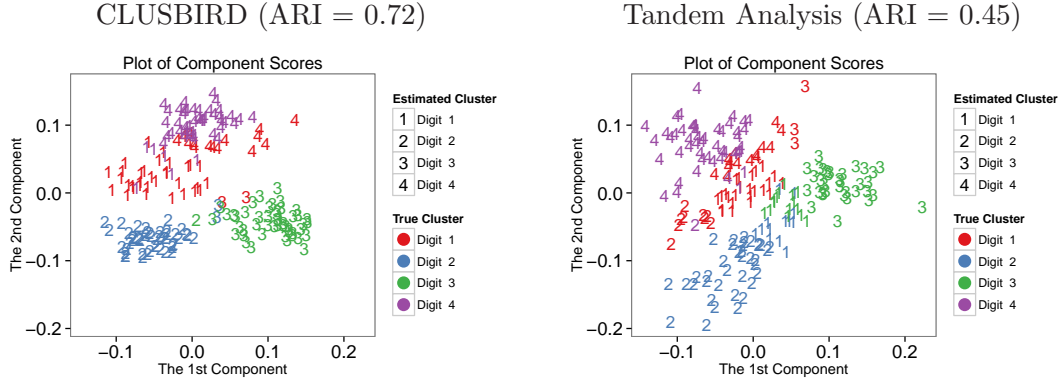


Figure 4: Plots of component scores estimated by CLUSBIRD and tandem analysis; in the plots, the number denotes the estimated cluster and the color denotes the true cluster

2013) which contains 5,620 objects. Each object represents one of the integers from 0 to 9, and we used images of 1, 2, 3, and 4, for which examples are shown in Figure 3. Each normalized bitmap includes a  $32 \times 32$  matrix, i.e., a 1,024-dimensional binary vector, in which each element indicates one pixel with a value of white or black. Fifty objects for each number were selected and thus  $50 \times 4 = 200$  objects were analyzed by the proposed method and tandem analysis with  $K = 4$  and  $L = 2$ . For the proposed method and the tandem approach, the value of a tuning parameter  $\lambda$  was determined by BIC.

Estimated component scores with clusters are shown in Figure 4. It can be seen that the proposed method provided a well-separated and compact low-dimensional cluster structure. On the other hand, tandem analysis provided crude recovery of the true cluster structure. In fact, the value of ARI for the proposed method was higher than that for tandem analysis. From this viewpoint, CLUSBIRD provided a better result than that of tandem analysis.

### 4.3 Population classification using single nucleotide polymorphism data

Association studies based on high-throughput single nucleotide polymorphism (SNP) data have become a popular way to detect genomic regions associated with complex human diseases. A crucial issue in association studies is population stratification detection (Hao et al., 2004), which is to determine whether a population is homogeneous or has hidden structures within it. With the presence of population stratification, a naive case-control approach that did not consider the stratification would yield biased results and, therefore, draw inaccurate scientific conclusions (Ewens and Spielman, 1995). We used the SNP dataset available in the International HapMap project (The International HapMap Consortium, 2005), filtering out those with minor allele frequencies greater than 0.01 and those missing genotype rates less than 0.05. The dataset consists of

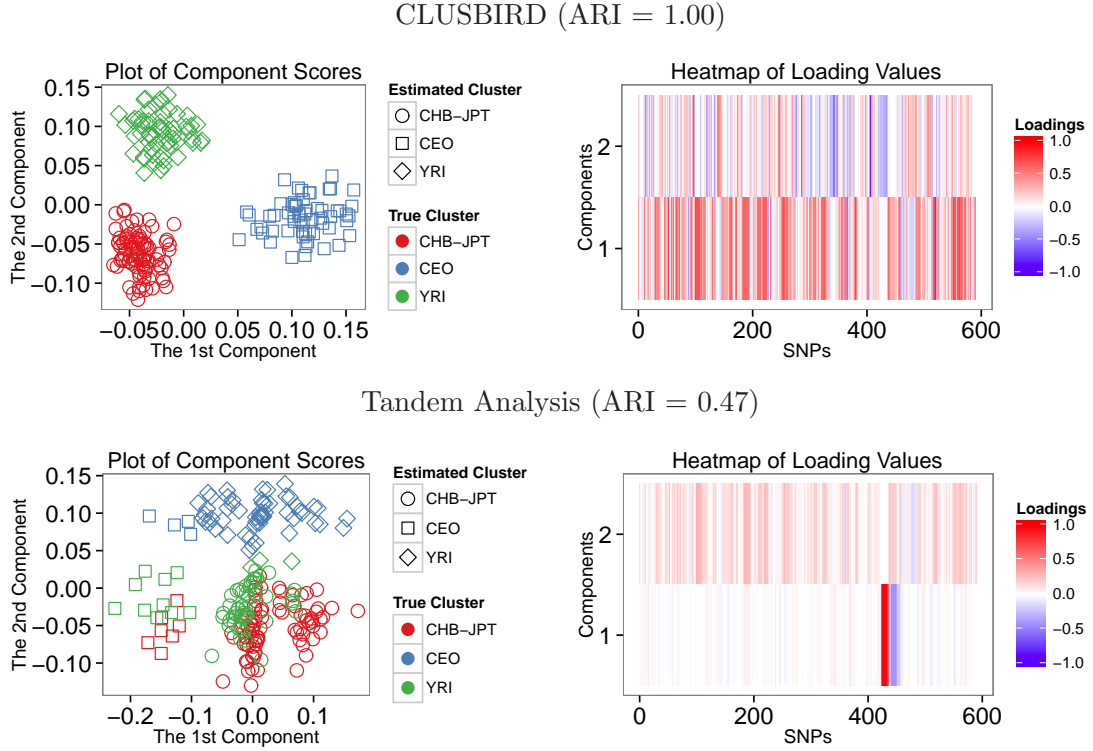


Figure 5: Plots of component scores (left) and loading values (right) estimated by CLUSBIRD and tandem analysis; in the left panel, the colors and shapes denote the true and estimated memberships, respectively; loading values were scaled so that the value existed in  $[-1, 1]$

3 different ethnic populations of 90 Asians (45 Han Chinese in Beijing, China; CHB and 45 Japanese in Tokyo, Japan; JPT), 60 Caucasians (Utah residents with ancestry from northern and western Europe; CEO), and 60 Africans (Yoruba in Ibadan, Nigeria; YRI). Here, we conducted the proposed method and tandem analysis to detect the three-subpopulation structure using the SNP data on the 210 subjects.

Since there were too many SNPs (2.2 million, 2.3 million, and 2.6 million SNPs for CHB-JPT, CEO, and YRI populations, respectively) to analyze those data, we had to select SNPs that were seen to be associated with detection of the subpopulation. First, using PLINK (Purcell, 2007), we conducted three association analyses in which each population was considered as a case and the other two populations were control. Then, we obtained SNPs which had genome-controlled p-values less than 0.1%. All those SNPs were considered to be related to the differences among the three ethnic populations. After selecting SNPs with no missing values, we finally obtained 589 SNPs of 210 subjects.

We conducted the proposed CLUBIRD method and tandem analysis with  $K = 3$  and  $L = 2$  using the SNP data. A tuning parameter was determined by BIC for both methods. The results are shown in Figure 5. We can see that the proposed method recovered the true ethnic populations perfectly. In contrast, tandem analysis provided a crude recovery of the populations. The tandem analysis, SLPCA, provided a bit sparse estimation of loading values, where only a few SNPs had large loading values for the first component and many SNPs had low loading values for the second component. Although this sparse structure may provide easy interpretation for the estimated low-dimensional structure, the structure did not contain the true ethnic populations well. The proposed method provided a reasonably sparse structure of loading values. Actually, all SNPs used for this analysis had some relation to detection of populations. Thus, it is reasonable that all SNPs had large loading values. In addition, for the proposed method, almost all SNPs had high loading values for one component, resulting in easy interpretation of the low-dimensional structure.

## 5 Conclusion

In this paper, we proposed a new procedure, called CLUBIRD, for simultaneously finding the optimal cluster structure for multivariate binary objects and finding the subspace to represent the cluster structure. The proposed method can provide the weight for each binary variable, which indicates the contribution of the variable to the cluster structure. In general, tandem analysis for clustering objects with dimension reduction is likely to fail in finding the cluster structure. In fact, our numerical examples demonstrate the inability of tandem analysis to detect the cluster structure and subspace for the structure. Those examples also show that our proposed method can provide a better cluster structure than tandem analysis. Furthermore, from the examples, we found that our procedure can work well for data that had a mildly larger number of variables than the sample size.

The proposed model can be considered an extension of the ordinary latent class analysis (LCA) (Aitkin et al., 1981). However, the ordinary LCA cannot provide loading values for variables and a low-dimensional structure. Also, LCA may not provide an appropriate estimation with the moderately high-dimensional dataset we used in the numerical examples. From this point of view, the proposed method can provide useful insight for researchers.

The proposed method can be extended to deal with various problems. For example, it is useful for the proposed model to deal with categorical variables, not just binary variables. In addition, the ordinary LCA model is ready for multi-group analysis, the analysis with covariates, and analysis of repeated measures data (Collins and Lanza, 2009). Using the formulation of LCA, the proposed model can also contain those features. These could be interesting topics for further research.

## Appendix A: Estimation of individual latent scores

To obtain individual component scores,  $\mathbf{G} = (g_{nl})$ , we propose a two-step approach. First, we estimate all parameters,  $\boldsymbol{\mu}$ ,  $\mathbf{A}$ ,  $\mathbf{F}$ , and  $\boldsymbol{\xi}$ , in the CLUSBIRD model. Then, we assume that a cluster structure of individuals is present in a low-dimensional space that is the same as that for the cluster center  $\mathbf{F}$ . That is, the estimated loading matrix  $\hat{\mathbf{A}}$  and low-dimensional centroids  $\hat{\boldsymbol{\mu}}$  also define the subspace for the individuals. Thus, we consider the following post hoc model. Suppose that  $\tilde{y}_{nd}$  ( $n = 1, \dots, N$ ;  $d = 1, \dots, D$ ) follows the Bernoulli distribution with success probability  $\pi_{nd} = \pi(\theta_{nd})$ , where  $\theta_{nd}$  is the logit transformation of  $\pi_{nd}$ . In addition, we assume that the canonical parameter  $\theta_{nd}$  has a low-rank representation

$$\theta_{nd} = \hat{\mu}_d + \mathbf{g}_n' \hat{\mathbf{a}}_d,$$

where  $\mathbf{g}_n = (g_{n1}, \dots, g_{nL})'$  with  $\mathbf{G}'\mathbf{G} = \mathbf{I}_L$ . Here, we write

$$S(\mathbf{G}) = \sum_{n=1}^N \sum_{d=1}^D \log \pi(q_{nd}(\hat{\mu}_d + \mathbf{g}_n' \hat{\mathbf{a}}_d)).$$

Then, we obtain individual component scores by maximizing  $S(\mathbf{G})$  over  $\mathbf{G}$ . Similar to the solution of  $\mathbf{F}$  in Section 3, the optimal  $\mathbf{G}$  can be obtained using the GP algorithm.

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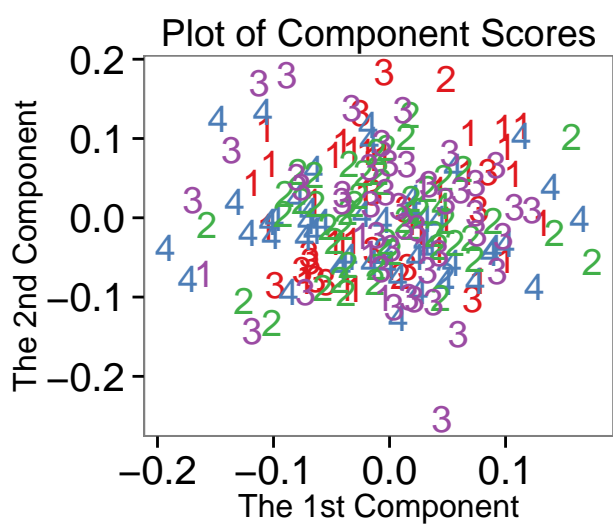
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Estimated Cluster

- |   |         |
|---|---------|
| 1 | Digit 1 |
| 2 | Digit 2 |
| 3 | Digit 3 |
| 4 | Digit 4 |

True Cluster

- |   |         |
|---|---------|
| ● | Digit 1 |
| ● | Digit 2 |
| ● | Digit 3 |
| ● | Digit 4 |

Loadings for the 1st Component

